

Study of the spin- $\frac{3}{2}$ Hubbard-Kondo lattice model by means of the Composite Operator Method

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Abstract

We study the spin- $\frac{3}{2}$ Hubbard-Kondo lattice model by means of the Composite Operator Method, after applying a Holstein-Primakov transformation. The spin and particle dynamics in the ferromagnetic state are calculated by taking into account strong on-site correlations between electrons and antiferromagnetic exchange among $\frac{3}{2}$ spins, together with usual Hund coupling between electrons and spins.

Key words: spin- $\frac{3}{2}$ Hubbard-Kondo lattice model, Composite Operator Method, Holstein-Primakov transformation

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The revival in the study of manganites has led to experimental re-examination of their different properties. One of the puzzling features is the strong deviation of the spin-wave dispersion from the typical Heisenberg behavior. In particular, it has been observed an unexpected softening at the zone boundary [1]. These observations are very important as they indicate that some aspects of spin dynamics in manganites have not been entirely understood yet [2,3]. According to this, we have decided to investigate the spin dynamics of the ferromagnetic state of the spin- $\frac{3}{2}$ Hubbard-Kondo lattice model by means of the Composite Operator Method (COM) [4]. The Hamiltonian under analysis reads as

$$H = \sum_{ij} (-2dt\alpha_{ij} - \mu\delta_{ij}) c^\dagger(i) c(j) + U \sum_i n_\uparrow(i) n_\downarrow(i) - J_H \sum_i \mathbf{s}(i) \cdot \mathbf{S}(i) + dJ_{AF} \sum_i \mathbf{S}(i) \cdot \mathbf{S}^\alpha(i) \quad (1)$$

where \mathbf{i} is a vector of the d -dimensional lattice and $i = (\mathbf{i}, t)$, μ is the chemical potential, $c^\dagger(i) = (c^\dagger_\uparrow(i), c^\dagger_\downarrow(i))$

is the electronic creation operator in spinorial notation, t is the hopping amplitude, α_{ij} is the nearest-neighbor projector, U is the on-site Coulomb interaction, $n_\sigma(i) = c^\dagger_\sigma(i) c_\sigma(i)$, J_H is the Hund coupling, $\mathbf{s}(i) = \frac{1}{2} c^\dagger(i) \boldsymbol{\sigma} c(i)$, $\boldsymbol{\sigma}$ are the Pauli matrices, $\mathbf{S}(i)$ is the core $\frac{3}{2}$ -spin, J_{AF} is the antiferromagnetic coupling. We have used the notation $\phi^\alpha(i) = \sum_j \alpha_{ij} \phi(\mathbf{j}, t)$.

In order to avoid the difficulties related to the high value of the core spin, we have used the Holstein-Primakoff transformation: $S_+(i) = \sqrt{2S - n_a(i)} a(i)$, $S_-(i) = a^\dagger(i) \sqrt{2S - n_a(i)}$, $S_z(i) = S - n_a(i)$, where $S = \frac{3}{2}$, $a(i)$ is a spinless bosonic destruction operator and $n_a(i) = a^\dagger(i) a(i)$. Then, we have decided to approximate the non-linear term $\sqrt{2S - n_a(i)}$ to the first order in $\frac{\delta n_a(i)}{2S - n_a}$ where $\delta n_a(i) = n_a(i) - \langle n_a(i) \rangle$ and $n_a = \langle n_a(i) \rangle$. It is worth noticing that this approximation preserves all properties related to the angular momentum algebra of the core spin. The transformed Hamiltonian reads as

$$H = \sum_{ij} (-2dt\alpha_{ij} - \mu\delta_{ij}) c^\dagger(i) c(j) + U \sum_i n_\uparrow(i) n_\downarrow(i) - J_H \sum_i [S - n_a - \delta n_a(i)] s_z(i)$$

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$$\begin{aligned}
& -\frac{1}{2}J_H A \sum_i \left[s_+(i) a^\dagger(i) \left(1 - \frac{\delta n_a(i)}{2A^2} \right) + h.c. \right] \\
& -2dJ_{AF} (S - n_a) \sum_i \delta n_a(i) \\
& + dJ_{AF} A^2 \sum_i a^\dagger(i) a^\alpha(i)
\end{aligned} \quad (2)$$

where $A = \sqrt{2S - n_a}$.

Within the framework of the COM, we have chosen two operatorial basis to study the spin and particle dynamics

$$B(i) = \begin{pmatrix} a(i) \\ s_+(i) \end{pmatrix} \quad \psi(i) = \begin{pmatrix} \xi_\uparrow(i) \\ \eta_\uparrow(i) \\ \xi_\downarrow(i) \\ \eta_\downarrow(i) \end{pmatrix} \quad (3)$$

where $\xi(i) = [1 - n(i)]c(i)$ and $\eta(i) = n(i)c(i)$.

Then, we have linearized the equations of motion by projecting the currents onto the basis

$$i \frac{\partial}{\partial t} B(\mathbf{i}, t) \cong \sum_j \varepsilon_B(\mathbf{i}, \mathbf{j}) B(\mathbf{j}, t) \quad (4)$$

$$i \frac{\partial}{\partial t} \psi(\mathbf{i}, t) \cong \sum_j \varepsilon_F(\mathbf{i}, \mathbf{j}) \psi(\mathbf{j}, t) \quad (5)$$

where

$$\varepsilon_{B,F}(\mathbf{i}, \mathbf{j}) = \sum_l m_{B,F}(\mathbf{i}, \mathbf{l}) I_{B,F}^{-1}(\mathbf{l}, \mathbf{j}) \quad (6)$$

$$m_B(\mathbf{i}, \mathbf{j}) = \left\langle \left[i \frac{\partial}{\partial t} B(\mathbf{i}, t) B^\dagger(\mathbf{j}, t) \right] \right\rangle \quad (7)$$

$$m_F(\mathbf{i}, \mathbf{j}) = \left\langle \left[i \frac{\partial}{\partial t} \psi(\mathbf{i}, t) \psi^\dagger(\mathbf{j}, t) \right] \right\rangle \quad (8)$$

$$I_B(\mathbf{i}, \mathbf{j}) = \left\langle \left[B(\mathbf{i}, t) B^\dagger(\mathbf{j}, t) \right] \right\rangle \quad (9)$$

$$I_F(\mathbf{i}, \mathbf{j}) = \left\langle \left[\psi(\mathbf{i}, t) \psi^\dagger(\mathbf{j}, t) \right] \right\rangle \quad (10)$$

This procedure assures that the neglected component of the current is orthogonal to the chosen basis. According to this, we have obtained the corresponding retarded Green's functions in the pole approximation

$$G_{B,F}(\omega, \mathbf{k}) = \sum_i \frac{\sigma_{B,F}^{(i)}(\mathbf{k})}{\omega - E_{B,F}^{(i)}(\mathbf{k}) + i\delta} \quad (11)$$

where the energies $E_{B,F}^{(i)}(\mathbf{k})$ are the eigenvalues of the energy matrices $\varepsilon_{B,F}(\mathbf{k}) = \mathcal{F}[\varepsilon_{B,F}(\mathbf{i}, \mathbf{j})]$ and the spectral densities $\sigma_{B,F}^{(i)}(\mathbf{k})$ can be computed in terms of the normalization matrices $I_{B,F}$ and of the eigenvectors of the energy matrices[4]. \mathcal{F} is the Fourier transform.

The parameters appearing in the expressions of $m_{B,F}$ and $I_{B,F}$ have the following definitions

$$n = \langle n(i) \rangle = 2 - (C_{F11} + C_{F22} + C_{F33} + C_{F44}) \quad (12)$$

$$m = \langle s_z(i) \rangle = \frac{1}{2} (C_{F44} - C_{F22}) \quad (13)$$

$$n_a = C_{B11} - 1 \quad (14)$$

$$\tilde{p}_1 = \frac{1}{m} (C_{F11}^\alpha + C_{F22}^\alpha + C_{F33}^\alpha + C_{F44}^\alpha) \quad (15)$$

$$\tilde{p}_2 = \frac{1}{A} \frac{\langle a(i) s_-(i) \rangle}{m} = \frac{1}{A} \frac{C_{B12}}{m} \quad (16)$$

$$\tilde{p}_3 = \frac{1}{A^2} \frac{\langle \delta n_a(i) s_z(i) \rangle}{m} \quad (17)$$

$$\tilde{p}_4 = \frac{1}{A^3} \frac{\langle \delta n_a(i) a(i) s_-(i) \rangle}{m} \quad (18)$$

$$\tilde{p}_5 = \frac{1}{A^2} \frac{\langle \delta n_a(i) n(i) \rangle}{m} \quad (19)$$

$$\Delta_0 = \frac{1}{2} (C_{F11}^\alpha - C_{F22}^\alpha + C_{F33}^\alpha - C_{F44}^\alpha) \quad (20)$$

$$\Delta_z = \frac{1}{2} (C_{F11}^\alpha - C_{F22}^\alpha - C_{F33}^\alpha + C_{F44}^\alpha) \quad (21)$$

$$\begin{aligned}
p = & \left\langle \left(\frac{1}{4} n^\alpha(i) n(i) + \mathbf{s}^\alpha(i) \cdot \mathbf{s}(i) \right) \right\rangle \\
& - \langle (c_\uparrow(i) c_\downarrow(i))^\alpha c_{\downarrow}^\dagger(i) c_{\uparrow}^\dagger(i) \rangle
\end{aligned} \quad (22)$$

$$\chi_z^\alpha = \langle n^\alpha(i) s_z(i) \rangle \quad (23)$$

where $C_{F\beta\gamma} = \langle \psi_\beta(\mathbf{i}) \psi_\gamma^\dagger(\mathbf{i}) \rangle$, $C_{F\beta\gamma}^\alpha = \langle \psi_\beta^\alpha(\mathbf{i}) \psi_\gamma^\dagger(\mathbf{i}) \rangle$ and $C_{B\beta\gamma} = \langle B_\beta(\mathbf{i}) B_\gamma^\dagger(\mathbf{i}) \rangle$. According to the prescriptions of the COM [4], the parameters that cannot be computed by their definitions (\tilde{p}_3 , \tilde{p}_4 , \tilde{p}_5 , p and χ_z^α) would be fixed by the following relations

$$C_{11} = C_{33} \quad C_{12} = 0 \quad (24)$$

$$C_{34} = 0 \quad C_{44} = C_{B22} \quad (25)$$

coming from the algebra and by one more relation coming from the request that the hydrodynamic limit should be satisfied (i.e., the existence of a sound mode). All these equations (definitions and constraints) form a coupled system that should be computed self-consistently. The results of these calculations will be presented elsewhere.

In conclusion, we have reported the solution for the Hubbard-Kondo model in presence of antiferromagnetic coupling between the core spin with the framework of the Composite Operator Method in the pole approximation. The model has been first mapped through the Holstein-Primakov transformation that has been then approximated to the first order in the number fluctuation operator. The spin dynamics has been fully determined and will be analyzed numerically.

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